

Orthoformic acid, cyclic 2,2-dimethyltrimethylene ethyl ester
5783-79-9 | DTXSID20206542

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 8.76 °C

Global applicability domain: Inside

Local applicability domain index: 5.92e-01

Confidence level: 6.18e-01

Nearest Neighbors from the Training Set

Image not found

Paraldehyde

Measured: 12.6

Predicted: 16.3

Image not found

1,1-Bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane

Measured: -30.0

Predicted: -17.6

Image not found

1,3,5-Triethoxybenzene

Measured: 43.5

Predicted: 43.1

Image not found

1,3,5-Trimethoxybenzene

Measured: 54.5

Predicted: 51.0

Image not found

1,3-Dioxane

Measured: -45.0

Predicted: -12.0